

Esol (pretrained)

GPR

GPT-InChI

GPT-SMILES

GPT-SELFIES

Weave

GraphConv

TabPFN

accuracy

0.4

0.2

F₁ macro

0.4

0.2

F₁ micro

0.4

0.2

κ

0.4

0.2

0.0

10

15

20

25

30

35

40

45

50

10

15

20

25

30

35

40

45

50

